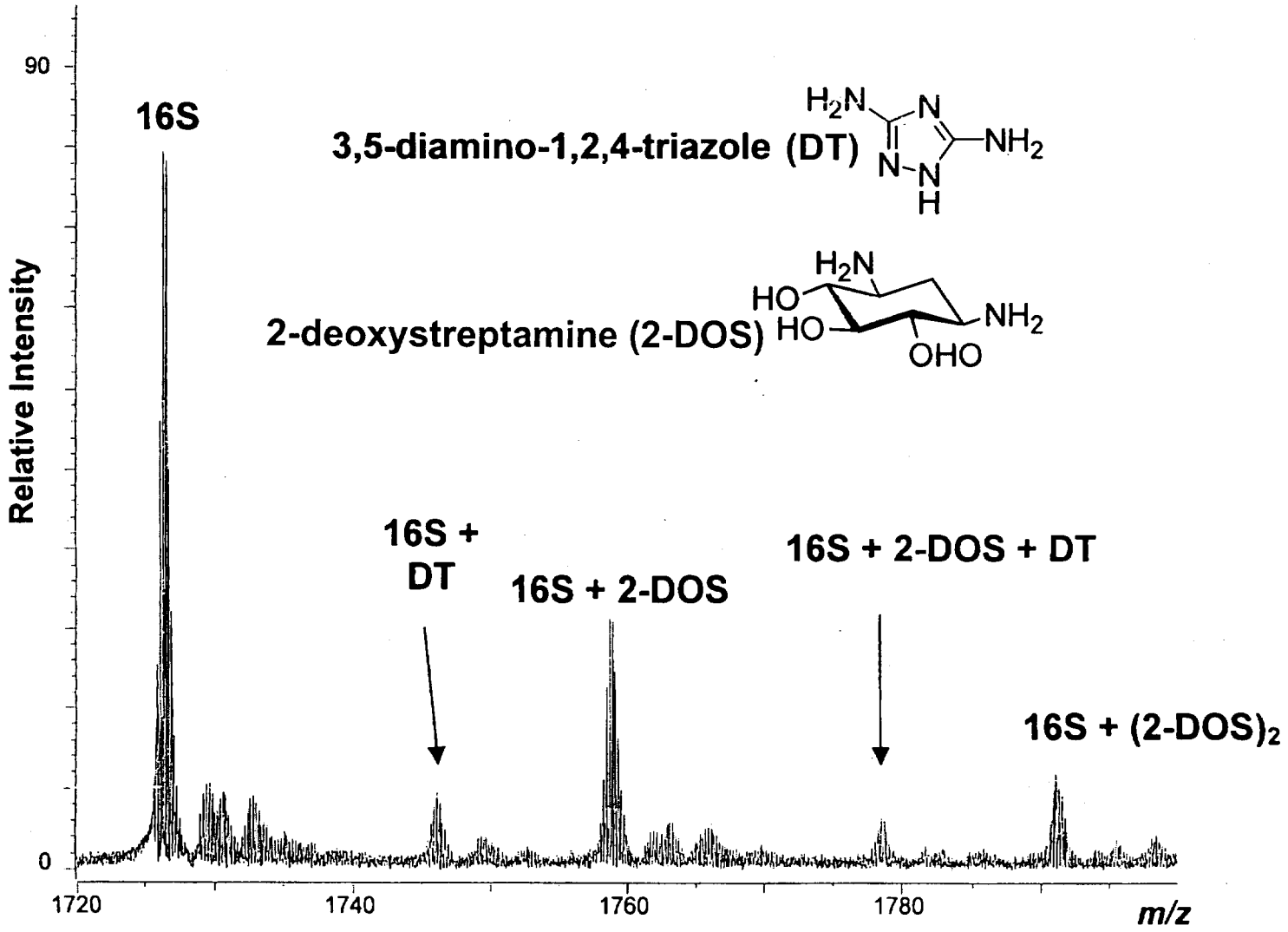
90
0
Relative Intensity
16S
3,5-diamino-1,2,4-triazole (DT)
2-deoxystreptamine (2-DOS)
16S + DT
16S + 2-DOS
16S + 2-DOS + DT
16S + (2-DOS)2
1720
1740
1760
1780
m/z

Figure 4

or

$$y = TL1L2 - 2 \times \frac{TL1 \times TL2}{T}$$

The above method for determining a concurrent binding interaction of two ligands is exemplified in figure 4 wherein 3,5-diamino-1,2,4-triazole (DT) and 2-deoxystreptamine (2-DOS) are both ligands for target RNA (a 27-mer fragment of ribosomal RNA comprising the 16S A-site). The mass-spectrum trace shows intensity signals for a ternary complex at approximately 1778 m/z for both ligands bound to the target 16S RNA, a binary complex at about 1758 m/z for 2-DOS bound to 16S RNA, a binary complex at 1746 m/z for DT bound to 16S RNA and another signal at about 1727 m/z for 16S RNA unbound by either ligand. The relative ion abundance of the ternary complex (16S+2-DOS+DT) with respect to the unbound 16S target RNA (16S) is equal, within limits of error, to the sum of the relative ion abundance of the contributing binary complex ((16S+DT) X (16S+2-DOS)) with respect to the unbound target (16S) and the contributing binary complex ((16S+2-DOS) + (16S+DT)) with respect to the unbound target (16S). Expressed in a simplified form of the formula:

$$y \approx (16S+2\text{-}DOS+DT) - 2 \times (16S+2\text{-}DOS) \times (16S+DT) / 16S$$

This indicates a concurrent binding interaction between the two ligands, 2-DOS and DT, for the target 16S RNA. Further, a comparison of the ion abundance of the two binary complexes indicates that 2-DOS has greater binding affinity for the target RNA than DT.